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Numerical Study of X-ray Spectroscopies for Understanding Anionic Redox in Li-ion Battery Compounds through Charge Transfer Hybridization Full Atomic Multiplet Theory ILKYU LEE, CHUNJING JIA, YVONNE KUNG, BRIAN MORITZ, TOM DEVEREAUX, Stanford Univ — The field of rechargeable batteries has gained incredible attention due to Lithium-ion transition metal compounds and their attractive properties such as high energy density and low self-discharge. Although the discovery of an anionic redox center in addition to the usual cationic redox led to a greater understanding of these battery compounds, the mechanism behind the anionic redox still remains unclear with various possible explanations. In this study, we utilize a first-principles approach combined with full charge transfer and atomic multiplet model to investigate different models of anionic redox by simulating x-ray spectra for Li-ion battery compounds. Through comparison with existing experimental data, we aim to achieve a greater understanding of the anionic redox process, in hopes of controlling the process and predicting novel, better performing Li-ion compounds.

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